




MACE: a Machine-learning Approach to Chemistry Emulation

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Summary

Astrochemistry is the study of chemical species in astrophysical objects. By combining observations and theoretical predictions, the physical conditions of the object can be analysed as well as its chemical composition and yields, since chemistry is closely coupled to the dynamics of the environment. Most often, such astrophysical environments are known to be complex and out of thermodynamic equilibrium. For that reason, the chemical evolution is usually modelled using the chemical kinetics approach, in which a set of non-linear coupled ordinary differential equations (ODEs) is solved for a given network of chemical species and reactions. For large chemical networks, however, this method is computationally slow. Therefore, we developed MACE, a *Machine-learning Approach to Chemistry Emulation*, inspired on similar work in the literature (e.g., Holdship et al. (2021); Grassi et al. (2022); Sulzer & Buck (2023)). MACE is a PyTorch module that offers a trainable surrogate model that is able to emulate chemical kinetics in a shorter computation time than its classical analogue. More specifically, it provides a machine learning architecture, consisting of an autoencoder and a trainable ODE, implemented in PyTorch and `torchode` (Lienen & Günemann, 2022). Mathematically, MACE is given by

$$\hat{n}(t) = \mathcal{D}\left(G(\mathcal{E}(\mathbf{n}, \mathbf{p}), t)\right), \quad (1)$$

where $\hat{n}(t)$ represents the predicted chemical abundances at time t , more details can be found in Maes et al. (2024) and in Fig. 1, which shows a schematic representation of the architecture and flow of the emulator. MACE is developed in the context of circumstellar envelopes (CSEs) of evolved stars, but is flexible to be retrained on data of other astrophysical environments.

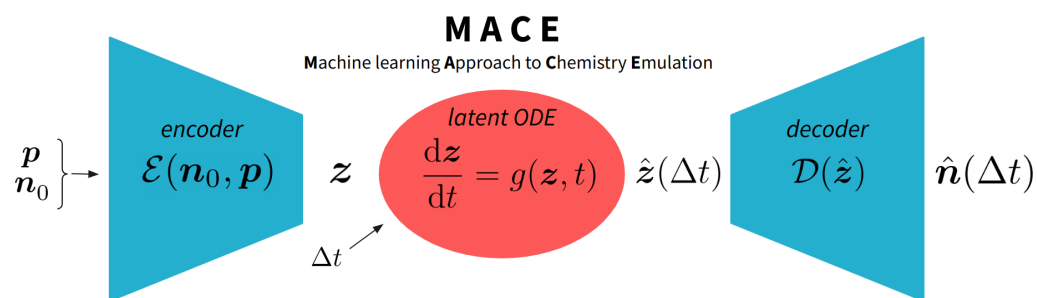


Figure 1: Schematic representation of the architecture of MACE. The symbols n and p represent the chemical abundances and physical parameters, respectively. The autoencoder (in blue) consists of an encoder \mathcal{E} , able to map n and p to a latent space representation z , and decoder \mathcal{D} , working the other way around. The function g represents the trainable ODE, which needs to be solved for a time step Δt . (Adapted from Maes et al. (2024).)

29 Statement of need

30 Astrophysical objects or environments entail 3D dynamical processes, as well as chemical
31 and radiation processes. Thus, in order to properly model such an environment, these three
32 constituents all need to be included in a single simulation. However, modelling each constituents
33 separately already poses a computational challenge for a modest parameter space, let alone
34 running a simulation with the three constituents integrated, and on an extended parameter
35 space. Specifically on the chemistry side, it is generally established that, from a mathematical
36 point of view, chemical kinetics is a stiff problem. When working with an extended chemical
37 network ($\gtrsim 100$ species, connected by $\gtrsim 1000$ reactions), the system becomes computationally
38 very slow to solve. Therefore, it is essential to speed up the solver in an alternative way,
39 also because the solver is applied multiple times when calculating the chemical evolution of
40 a certain environment. A fast and accurate chemistry solver would make it computationally
41 feasible to run it alongside a 3D hydrodynamical and/or radiation model.

42 Example case

43 In the context of circumstellar envelopes, we aim to build a comprehensive model, consisting of
44 3D hydrodynamics, chemistry, and radiation. This is needed since recently, complex structure
45 (such as spiral, arcs, and bipolarity) are observed in CSEs around evolved, low- and intermediate
46 mass stars, currently attributed to the presence of (sub-)stellar companions (Decin et al., 2020;
47 Gottlieb et al., 2022; Nordhaus & Blackman, 2006). In order to study these stars and their
48 CSEs, taking into account companions, accurate 3-dimensional models are needed. Currently,
49 only hydrodynamical modelling is done for these systems in 3D (e.g., Maes et al. (2021);
50 Malfait et al. (2021)), though the aim is to include chemistry as well as radiation (Maes et al.,
51 2022). Starting with integrating chemistry and 3D hydrodynamics, this coupling will only be
52 computationally feasible when a faster alternative to chemical kinetics exists.

53 The development of MACE is a first step towards this coupling. Using the MACE architecture,
54 we are able to reproduce the 1D abundance profiles of 468 chemical species with an accuracy
55 between 10 and 18, averaged over 3000 tests, for MACE models with different sets of
56 hyperparameters, for the following error metric:

$$\text{error} = \frac{\log_{10} n - \log_{10} \hat{n}}{\log_{10} n}, \quad (2)$$

57 which is executed element-wise and subsequently summed over the different chemical species.
58 More details on the accuracy of the MACE models can be found in Maes et al. (2024). Fig.
59 2 shows the abundance profiles of seven chemical species, where the full curves indicate the
60 MACE test of model *int4* from Maes et al. (2024), and the dashed curves give the result for
61 the classical model. On average, the MACE routine provides a speed-up of a factor 26, not
62 taking into account the potential extra speed-up factor due to efficient vectorisation when
63 coupling MACE with an SPH hydrodynamical model.

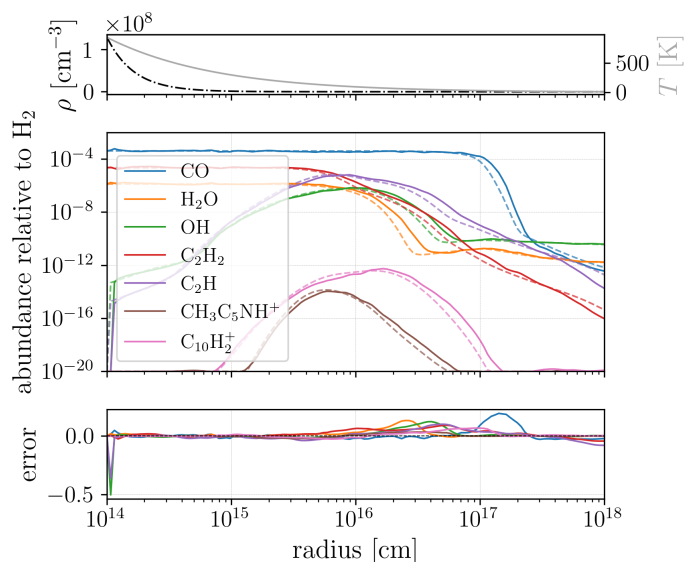


Figure 2: Chemical abundance profiles from a test of trained MACE model model *int4* (full curves), compared to the classical model (dashed curves). The error on the MACE model is calculated according to Eq. (2). More details in Maes et al. (2024).

64 Code availability

65 The code of MACE is publicly available in a GitHub repository: <https://github.com/silkemaes/MACE>.
66

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76 METH24/012.

77 References

78 Decin, L., Montargès, M., Richards, A. M. S., Gottlieb, C. A., Homan, W., McDonald, I., El
79 Mellah, I., Danilovich, T., Wallström, S. H. J., Zijlstra, A., Baudry, A., Bolte, J., Cannon,

- 80 E., De Beck, E., De Ceuster, F., de Koter, A., De Ridder, J., Etoke, S., Gobrecht, D.,
81 ... Yates, J. (2020). (Sub)stellar companions shape the winds of evolved stars. *Science*,
82 369(6510), 1497–1500. <https://doi.org/10.1126/science.abb1229>
- 83 Gottlieb, C. A., Decin, L., Richards, A. M. S., De Ceuster, F., Homan, W., Wallström, S. H.
84 J., Danilovich, T., Millar, T. J., Montargès, M., Wong, K. T., McDonald, I., Baudry, A.,
85 Bolte, J., Cannon, E., De Beck, E., de Koter, A., El Mellah, I., Etoke, S., Gobrecht, D., ...
86 Zijlstra, A. (2022). ATOMIUM: ALMA tracing the origins of molecules in dust forming
87 oxygen rich M-type stars. Motivation, sample, calibration, and initial results. *660*, A94.
88 <https://doi.org/10.1051/0004-6361/202140431>
- 89 Grassi, T., Nauman, F., Ramsey, J. P., Bovino, S., Picogna, G., & Ercolano, B. (2022).
90 Reducing the complexity of chemical networks via interpretable autoencoders. *668*, A139.
91 <https://doi.org/10.1051/0004-6361/202039956>
- 92 Holdship, J., Viti, S., Haworth, T. J., & Ilee, J. D. (2021). Chemulator: Fast, accurate
93 thermochemistry for dynamical models through emulation. *653*, A76. <https://doi.org/10.1051/0004-6361/202140357>
- 95 Lienen, M., & Günnemann, S. (2022). Torchode: A parallel ODE solver for PyTorch. *The*
96 *Symbiosis of Deep Learning and Differential Equations II, NeurIPS*. <https://openreview.net/forum?id=uiKVKTiUYB0>
- 98 Maes, S., De Ceuster, F., Van de Sande, M., & Decin, L. (2024). MACE: A Machine
99 learning Approach to Chemistry Emulation. *arXiv e-Prints*, arXiv:2405.03274. <https://doi.org/10.48550/arXiv.2405.03274>
- 101 Maes, S., Homan, W., Malfait, J., Siess, L., Bolte, J., De Ceuster, F., & Decin, L. (2021). SPH
102 modelling of companion-perturbed AGB outflows including a new morphology classification
103 scheme. *653*, A25. <https://doi.org/10.1051/0004-6361/202140823>
- 104 Maes, S., Siess, L., Homan, W., Malfait, J., De Ceuster, F., Ceulemans, T., Donné, D.,
105 Esseldeurs, M., & Decin, L. (2022). Route towards complete 3D hydro-chemical simulations
106 of companion-perturbed AGB outflows. In L. Decin, A. Zijlstra, & C. Gielen (Eds.), *The*
107 *origin of outflows in evolved stars* (Vol. 366, pp. 227–233). <https://doi.org/10.1017/S1743921322000217>
- 109 Malfait, J., Homan, W., Maes, S., Bolte, J., Siess, L., De Ceuster, F., & Decin, L. (2021).
110 SPH modelling of wind-companion interactions in eccentric AGB binary systems. *652*, A51.
111 <https://doi.org/10.1051/0004-6361/202141161>
- 112 Nordhaus, J., & Blackman, E. G. (2006). Low-mass binary-induced outflows from asymptotic
113 giant branch stars. *370*(4), 2004–2012. <https://doi.org/10.1111/j.1365-2966.2006.10625.x>
- 114 Sulzer, I., & Buck, T. (2023). Speeding up astrochemical reaction networks with autoencoders
115 and neural ODEs. *arXiv e-Prints*, arXiv:2312.06015. <https://doi.org/10.48550/arXiv.2312.06015>
116 06015